Original
multiple Inerts
+ PC Codes
PC - 999999
general inerts

UNITED STATES ENVIRONMENTAL PROTECTION AGENCY
WASHINGTON, D.C. 20460

OFFICE OF
PREVENTION, PESTICIDES AND
TOXIC SUBSTANCES

Date: May 15, 2002

MEMORANDUM

SUBJECT: Tolerance Review of Compounds Known as Fatty Acids, Fatty Acid Salts, and Fatty Acid Esters, and Fatty Acid Derivatives Classified as Inert Ingredients in Terrestrial and/or Aquatic Agricultural and Non-Agricultural Uses

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This Memorandum transmits the environmental fate, exposure, and ecotoxicity assessments performed by the Environmental Fate and Effects Division (EFED) for the fatty acids, fatty acid salts, fatty acid esters, and fatty acid derivatives classified as "Inerts". The assessments were performed based on readily available information form the Agency, peer-reviewed, open scientific literature, and Structure Activity Relationships (SAR). The information gathered from these sources allows EFED to conduct these environmental fate, exposure, and ecotoxicity assessments for these chemical compounds.

If you should have any questions concerning these sources of information and the assessments, please contact Silvia Termes at 305-5243 or Henry Craven and 305-5320.

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Conclusions

A review of the readily available information and Structure-Activity Relationships (SAR) on the compounds listed as "fatty acids, salts, esters, and other derivatives" is sufficient to perform a qualitative assessment of the fate and exposure in the environment and the ecotoxicity of these families of chemical compounds. In pesticides, these chemicals may be used in the formulation of products and/or in tank mixes. However, all of these compounds are widely used at an industrial scale and/or used for human consumption. In addition, many of them are found in nature as plants and animal fats and oils, from which they are liberated by hydrolysis. Therefore, their occurrence in nature and wide industrial are largely responsible for environmental loading. Fatty acids can be commercially obtained from tallow, coconut, soybean, tall oil, and from paraffin oxidation.

Fatty acids are carboxylic acids containing long, aliphatic carbon chains. It is the structural features of fatty acids that define the physical and chemical behavior of these compounds. The long carbon chain provides a hydrophobic (lipophilic) end, generally referred as the "hydrophobic tail" whereas the carboxylic acid constitutes the polar, hydrophilic (lipophobic) headgroup. The hydrophobic end interacts with hydrophobic substances while the hydrophilic group interacts with hydrophilic substances, in a "like-dissolves-like" manner. All of the"fatty acids" (free, salts, esters, and other derivatives) used as inerts have a straight-chain (i.e. no branching) tail. The hydrophobic tail can be either saturated or unsaturated (one or more carbon-to-carbon double bonds). Among the most common saturated fatty acids tails listed as inerts come from palmitic and stearic acids. Unsaturated fatty acid "inerts" come from oleic, linoleic, and linolenic acids.

Microbial degradation is the major route of transformation in the environment. Adsorption onto soil and sediment particulates is strong and, therefore, there is no potential to reach surface water by dissolved runoff and/or leach to surface water. Volatilization from soils and water is not likely to be a transport process in the environment. Although the potential to bioaccumulate is high, bioavailability is offset by the tendency to adsorb strongly to soil and sediment particulates. However, concentration at the water-air interface is likely to be higher than in the water column, which results in lowering the surface tension of the aqueous system. The lowering of the surface tension and the hydrophobic layer at the water-air interface has the potential to alter the physical and chemical characteristics of the aquatic environment. Detections in water resources (non-quantified) have been associated with areas that produce or consume large amounts of fatty acid products, such as in olive oil producing areas.

Introduction

All of the "fatty acid inerts" (fatty acids, fatty acid esters, fatty acid salts, and other fatty derivatives) were evaluate as a group, as the physical, chemical, and environmental behavior is dominated by the fatty acid groups. Thus, this risk assessment applies to all of the fatty inerts and took into consideration not only the length and saturation of the acid fatty hydrophobic chain, but also the nature of the headgroup. The assessments used data from the open literature or estimated using the Estimation Program Interface, Version 3.10 (EPI). Physical, chemical, environmental, and ecotoxicity data are presented in Tables 1 through 6. The tables were organized as follows:

Table 1 **Fatty Acids (Free Acids), C8- C14 (Saturated)**.Other fatty acids included under "Fatty acids, conforming to 21 CFR 172.860" besides palmitic, stearic, and oleic acids. Caprylic Acid (C8; CAS Reg.No. 124-07-10), Capric acid (C10; CAS Reg. No.334-48-5), Lauric acid (C12; CAS Reg.No.143-07-7), and Myristic acid (C14: CAS Reg. No. 544-63-8).

Table 2- **Fatty Acids (Free Acids), C16- C18 (saturated) and C18 (unsaturated).** Included in this table are the saturated chain Palmitic (C16; CAS Reg.No. 57-10-3) and Stearic (C8; CAS Reg No. 57-11-4) acids and the monounsaturated chain Oleic acid (C18; CAS Reg. No. 112-80-1)

Table 3- **Fatty Acid Esters**. Included in this table are the saturated-chain Isopropyl Myristate (C14; CAS Reg. No. 110-27–0) and Butyl stearate (C18; CAS Reg. No. 133-95-5)(C14-C18 and the monosaturated chain Methyl oleate (C18; CAS 112-62-9). Also included in this table is Ascorbyl palmitate (C16; CAS Reg. No. 136-66-6) and Glyceryl Monostearate (31566-31-1)

Table 4- **Derivatives of Fatty Acids (Non-Esters).** Included here is the monounsaturated-chain Sodium oleyl sulfate (C18: CAS Reg. No. 1847-55-8)

Table 5- **Alkali Metal, Alkali Earth, and Ammonium Salts of Fatty Acids**. Included here are Potassium Laurate (C12; CAS Reg. No. 10124-65-9), Magnesium stearate (C18; CAS Reg. No. 557-04-0) and Calcium stearate (C18; CAS Reg. No. 1592-23-0), and Ammonium stearate (C18; CAS Reg . No. 1002–89-7). to 21 CFR 172.863".

Table 6- **Aluminum and Zinc Stearates.** Aluminum (C18; CAS Reg. No. 637-12-7) and Zinc (C18; CAS Reg. No. 557-08-1) stearates were included in this table because they are included under "Salts of fatty acids, conforming to 21 CFR 172.863" and "Zinc stearate, conforming to CFR 182-5994).

A. Environmental Transformation and Transport

<u>Physical/and chemical properties and environmental fate behavior: Structure-Activity Relationships</u>

Physical and Chemical Properties

The length of the chain and degree of saturation, as well as the nature of the headgroup, define the physical and chemical properties, and subsequently influence the environmental behavior and interaction with organisms.

Physical and Chemical Properties and their Environmental Implications

Physical and Chemical Property	Environmental Fate and Biological Interactions
Solubility in water; pKa	Determines concentration in aqueous media. The solubility of saturated fatty acids decrease with the number of carbon atoms in the chain. Fatty acids, esters, salts, and other derivatives are surface active agents (surfactants). Strictly speaking, surfactants are not found in solution as discrete molecules, but in clusters (miscelles). In aqueous media, the hydrophobic group are oriented towards the center of the miscelle and the polar groups outside the miscelle. The pKa of fatty acids range from 4 to 5.5 and, therefore, are predominantly present as the anion in natural waters and biological systems.
n-octanol/water partition coefficient, as Kow or logKow	The higher the Kow/log Kow, the higher the hydrophobicity of the chemical and the higher the tendency to bioccumulate
K_{oc}	The higher the K_{oc}, the stronger the chemical adsorbs onto soils and sediment and the lower partitioning into the aqueous phase
Vapor pressure	The higher the vapor pressure, the higher the tendency to volatilize from soils
Henry's Law Constant	The higher the tendency to volatilize from water, the lowest the concentration in aqueous media

One of the major properties of surfactants in general is to reduce the interfacial air-water tension (surface tension). At the air-water interface, the hydrophobic tails are oriented towards the air phase, displacing water molecules at the interface and creating a hydrophobic environment at the water surface. Even though this has the potential to modify the aquatic environment, it is more likely to be caused by uses other than pesticides, except in areas where use of these compounds is the sole source of environmental loading. In addition, in natural water systems micelle formation (see "Solubility") is also influence by the "hardness" of the water. The presence of calcium and magnesium ions in "hard waters" precipitate the highly insoluble calcium and magnesium salts.

Transformation and Transport in the Environment

Microbial degradation is the major route of transformation in the environment. Adsorption onto soil and sediment particulates is strong and, therefore, there is no potential to reach surface water by dissolved runoff and/or leach to surface water. Volatilization from soils and water is not likely to be a transport process in the environment. Although the potential to bioaccumulate is high, bioavailability is offset by the tendency to adsorb strongly to soil and sediment particulates. However, concentration at the water-air interface is likely to be higher than in the water column.

Fatty Acid Inerts- Environmental Transformation and Transport

Environmental Process	Structural Characteristics and Properties of the Compounds	Implications/Conclusions
Hydrolysis	The ester bond is susceptible to hydrolysis, predominantly based-catalyzed.	Only the fatty acid esters undergo hydrolysis. Hydrolysis is faster at alkaline pH and slower at neutral and acid pH ,but even in alkaline pHs it is still slow (4-months or over). See Table
Photolysis	No chromophores in the 290 to 800 nm range (sunlight) indicate that <u>direct</u> photolysis is not a transformation pathway. However, indirect photolysis might be a potential transformation pathway via singlet oxygen. No data is available to assess the contribution of indirect photolysis in the environment	Direct photolysis is not a transformation process
Biodegradation	**Biodegradation is the key route of transformation in the environment**. Both chain length and nature of the headgroup. Although data on biodegradation under anaerobic conditions is scarce, there are indications that biodegradation under anaerobic conditions is slower than under aerobic conditions	According to the information compiled for the fatty acids, esters of fatty acids, fatty acid salts, and other fatty derivatives, biodegradation range between 3 weeks to 4 days Concentrations may be higher in anoxic than in oxic water systems

Environmental Process	Structural Characteristics and Properties of the Compounds	Implications/Conclusions
Sorption	Adsorption onto soil and sediment particulates is generally strong. It depends on concentration in the aqueous phase, ratio of water volume to water-solid interface, and sorption is generally non-linear (i.e., Freundlich isotherms are non-linear and 1/n deviates from the accepted 0.9 tp 1.1 range for linear absorption) Generally, adsorption is stronger with increasing carbon chain length. However, the headgroup is also important. For example, the amphoteric L-ascorbyl palmitate does not adsorb strongly to soils when compare to other fatty acid compounds	Adsorption to soils and sediments, rather than partitioning into the water column, decreases bioavailability in aquatic ecosystems. However, there is the potential that a hydrophobic layer may be present at the water-air interface In "hard waters" (calcium and magnesium rich), fatty acids precipitate as the highly insoluble calcium and magnesium salts In the environmentally significant pH range of 5 to 9, fatty acids predominate in the anion form. Anions are generally more mobile than the acid. Although no K_{oc} estimates have been performed for the anionic form, it has been speculated that adsorption would be also strong
Volatilization	Low vapor pressure/Henry's Law constants are generally estimated. However, estimates suggest that there is a low potential for volatilization from soil and water	Volatilization may not be a transport process
Bioaccumulation	The high *n*-octanol-water partition coefficients suggest a high potential for bio- accumulation by aquatic organisms	Sorption to soils and sediments reduce bioavailabiltiy in aquatic media, thus competing with the potential for bioaccumulation. Most fatty acids are extensively metabolized by organisms

Fatty Acids (Free Acids), C8- C14 (Saturated)

As a group these compounds show the following trends with increasing chain length: decreasing water solubility, decreasing potential for volatilization, greater likelihood to partition and bind to soil and or sediment. Volatility from soil and water (Henry's Law Constant) and microbial mediated degradation are expected to limit transport to surface and ground water from applications or releases to land, with biodegradation being the major route of environmental dissipation. The only ecotoxicity data for this group of fatty acid is limited to estimated 14 day LC50 data on fish (Table

1). The toxicity ranges from moderately toxic (4.02 ppm) for the C10 to highly toxic (0.1 ppm) for the C14. Although the 96 hour LC50 values will be higher, that is appears to be less toxic then the 14 day values, without more information, it is not possible to categorize the acute toxicity based on a 96 hour exposure period. In conclusion these compounds, notably the C12 and C14, are not likely to be found in water at concentrations that would cause acute risk to fish.

Fatty Acids (Free Acids), C16- C18 (saturated) and C18 (unsaturated)

The only ecotoxcity data for this group of fatty acid is limited to estimated 14 day LC50 data on fish and the rat acute oral(Table 1). Based on this limited data set (toxicity ranges from 0.02 to 0.004 ppm), these compounds appear to be very highly toxic to fish. The 96 hour LC50 values will be higher, that is appears to be less toxic then the 14 day values, but without more information, it is not possible to categorize the acute toxicity based on a 96 hour exposure period. Although this group of fatty acids is more toxic to fish then the C8 -- C14 free acids, they are far less mobile, are bound more tightly to sediment and their water solubility and tox values are much closer to one another (ie. Palmitic acid has a water solubility of 0.04 ppm and a 14 day LC50 value of 0.02) such that the potential risk to fish should be less then the C8--C14. Terrestrial animal toxicity based on available rat data would indicate the 16 through C18 free acids are practically non-toxic on an acute basis.

Fatty Acid Esters.

Estimated ecotoxicity data for aquatic plants and animals and one rat acute oral are available (Table 3). Acute toxicity estimates range from moderately toxic (1.2 ppm) to very highly toxic (0.004 ppm) for fish; highly toxic (0.36 ppm) to very highly toxic (2.6×10^{-5} ppm) for *Daphnia magna*; and 0.04 to 4×10^{-4} ppm for green algae. Chronic toxicity estimates for fish range from 0.012 to 8.5×10^{-6} ppm. Based on a comparison of the 96 hour fish LC50 values of this group of fatty acids with the two free acid groups it appears that this group potentially more toxic than the free acid groups. However, for the 5 compounds and their derivatives that are included in this group, the water solubility is less than the estimated fish 96 hour LC50s. Considering this factor and in combination with the very low mobility and bioavailability there is less potential for acute risk to fish than for the free acid groups. Aquatic invertebrates will be at greater acute risk than fish, nevertheless the greatly reduced bioavailability and fairly rapid microbial degradation – approximately 4 days for primary degradation – will not likely result in a significant risk. The one available rat acute oral study is on Ascorbyl Palmitate (C16). Although this compound was the most toxic to aquatic organisms of the 5 compounds in this group, since the material is practically non toxic to mammals, this suggests that the 4 other compounds may be even less of a concern to terrestrial vertebrates.

Derivatives of Fatty Acids (Non-Esters)

The ecotoxicity data found in Table 4 is limited to a single 14 day fish LC50 for one of the two compounds in this group. The 96 hour LC50 would be no more than moderately toxic because it would be a higher value than the 14 day value of 3.88 ppm. Based on the compound's low mobility and bioavailability; fairly rapid microbial degradation (3.6 days); plus the water solubility being less than the estimated fish LC50 value there appears to be little potential for acute risk.

Alkali Metal, Alkali Earth, and Ammonium Salts of Fatty Acids

This collection of compounds does not constitute a homogenous group as evidenced by the chemistry and ecotox data included in Table 5. Acute toxicity estimates range from a 14 day LC50 of 1625 ppm (practically non toxic) to 1.13×10^{-9} ppm (very highly toxic) for fish; 48 hour EC50s of 2.77 and 2.84×10^{-9} ppm (very highly toxic) for *Daphnia magna*; 96 hour EC50 3.5 and 3.6×10^{-9} ppm for green algae and 96 hour LC50 4.75 and 4.88×10^{-14} ppm (very highly toxic) for estuarine invertebrates. The estimated 30 day chronic fish value is 1.04×10^{-9} ppm. Except for the estuarine invertebrate – mysid shrimp– the acute and chronic tox values are higher than the water solubility. Although mysids may be at greater risk than other aquatic organisms, nevertheless the extreme immobility, high binding and rapid microbial degradation will likely mitigate any potential for risk. Based solely on a single acute oral LD50 to bobwhite quail with a 14 % formulation of ammonium stearate (2,150 mg/kg) these compounds may be practically non toxic to terrestrial vertebrates.

Aluminum and Zinc Stearates

When compared to the 5 other groups into which the fatty acids have been placed, these two compounds are the least water soluble and mobile and most tightly bound to sediment. The EPI program estimated biodegradation to occur at the same rate (approximately 3.5 days) as most other fatty acids under review. In addition to the chemistry data, Table 6 includes the ecotox data. Acute toxicity values are 96 LC50 9.5×10^{-10} and 2.3×10^{-17} ppm (very highly toxic) for fish; 48 hour EC50s of 2.4×10^{-9} and 1.0×10^{-16} ppm (very highly toxic) for *Daphnia magna*; 96 hour EC50 3.5×10^{-9} and 2.1×10^{-16} ppm for green algae and 96 hour LC50 4.75×10^{-14} and 2.6×10^{-24} ppm (very highly toxic) for estuarine invertebrates. The estimated 30 day chronic fish value is 8.37×10^{-17} ppm. Except for the estuarine invertebrate – mysid shrimp– the acute and chronic tox values are higher than the water solubility. Although mysids may be at greater risk than other aquatic organisms, nevertheless the extreme immobility, high binding and rapid microbial degradation will likely mitigate any potential for risk. Based solely on a single acute oral LD50 to rats with zinc stearate (>10,000 mg/kg) these compounds may be practically non toxic to terrestrial vertebrates.

Sources of Information

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Table 1 Fatty Acids (Free Acids), C8- C14 (Saturated)

Physical and Chemical Property	Caprylic Acid (C8) [1] Octanoic acid 124-07-02	Capric Acid (C10) [1] Decanoic Acid 334-48-5	Lauric Acid (C12) [1] Dodecanoic Acid 143-07-7	Myristic Acid (C14) [1] Tetradecanoic 544-63-8
Number of carbon double bonds	None	None	None	None
Water Solubility, mg/L	789, experimental (30° C)	61.8, experimental (25° C)	4.81, experimental (25° C)	1.07, experimental (25° C)
Vapor Pressue, mmHg	3.7×10^{-3}, experimental (25° C)	3.7×10^{-4}, experimental (25° C)	1.6×10^{-5}, experimental (25° C)	1.4×10^{-5}, experimental (25° C)
Henry's Law Constant, atm-m^3/mole	8.9×10^{-7} experimental (25° C)	1.3×10^{-6}, experimental (25° C)	9.3×10^{-6}, experimental (25° C)	4.9×10^{-7}, experimental (25° C)
Log Kow	3.05, experimental	4.9, experimental (25° C)	4.6, experimental (25° C)	6.1, experimental
K_{oc}	25.62	87.16	296.5	1009
Hydrolysis Photolysis	Stable to hydrolysis and direct photolysis in water	Stable to hydrolysis and direct photolysis in water	Stable to hydrolysis and direct photolysis in water	Stable to hydrolysis and direct photolysis in water
Biodegradation (Expert Survey)	Ultimate (weeks) 3.5 Primary (days) 4.3	Ultimate (weeks) 3.4 Primary (days) 4.3	Ultimate (weeks) 3.4 Primary (days) 4.2	Ultimate (weeks) 3.4 Primary (days) 4.2
Fish Acute Toxicity, 14 day-LC_{50}, ppm	No ecotoxicity data found in ECOSAR	neutral organic (4.02)	neutral organic (0.66)	neutral organic (0.10)

[1] Other fatty acids included under "Fatty acids, conforming to 21 CFR 172.860" besides palmitic, stearic, and oleic acids

Table 2- Fatty Acids (Free Acids), C16- C18 (saturated) and C18 (unsaturated)

Physical and Chemical Property	Palmitic Acid (C16) Hexadecanoic Acid 57-10-3	Stearic Acid (C18) Octadecanoic Acid 57-11-4	Oleic Acid (C18) 9-Octadecanoic Acid, *Z*- 112-80-1	"Tall oil" 8002-26-4, 61790-12-3, 68647-71-2, 8052-10-6 Not located in EPI or ECOSAR
Number of carbon double bonds	None	None	One Can exist as *cis*- and *trans*-isomers	
Water Solubility, mg/L	0.04, experimental (25° C)	3.5×10^{-3}, experimental (25° C)	0.011, experimental (25° C)	
Vapor Pressure, mmHg	3.8×10^{-7}, experimental (25° C)	7.2×10^{-7}, experimental (25° C)	1.4×10^{-6}, experimental (25° C)	
Henry's Law Constant, atm-m^3/mole	2.5×10^{-7} experimental (25° C)	4.7×10^{-7}, experimental (25° C)	1.66×10^{-3}, EPI-estimated (25° C)	
Log Kow	7.7, experimental	8.3, experimental (25° C)	7.64, experimental (25° C)	
K_{oc}	3431	11,670	11,000	
Hydrolysis Photolysis	Stable to hydrolysis and direct photolysis in water	Stable to hydrolysis and direct photolysis in water	Stable to hydrolysis, and direct photolysis in water	
Biodegradation (Expert Survey)	Ultimate (weeks) 3.3 Primary (days) 4.1	Ultimate (weeks) 3.2 Primary (days) 4.1	Ultimate (weeks) 3.2 Primary (days) 4.1	
Fish Acute Toxicity, 14 day-LC_{50}, ppm	neutral organic (0.02)	neutral organic (0.003)	neutral organic (0.004)	
Mammal, acute oral LD50 mg/kg	>10,000		74,000	

Table 3- **Fatty Acid Esters (C14- C18 fattyacids ; Saturated) and C-18 fatty acid, Unsaturated**

Physical and Chemical Property	Isopropyl Miristate (C14) Tetradecanoic Acid, 1-methylethyl ester 110-27-0	Ascorbyl Palmitate (C16) L-Ascorbic acid, 6-hexadecanoate 137-66-6	Butyl Stearate (C18) Octadecanoic Acid, butyl ester 123-95-5	Methyl Oleate (C18) 9-Octadecenoic Acid (*Z*)-, methyl ester 112-62-9
Number of carbon double bonds	None	None	None	One Can exist as *cis*- and *trans*-isomers
Water Solubility, mg/L	0.013, experimental (30° C)	0.06, experimental (25° C)	3.64×10^{-5}, experimental (25° C) EPI estimated 3.64×10^{-5}, which is more in line with the longer-chain fatty acid esters	5.6×10^{-3} experimental (25° C)
Vapor Pressure, mmHg	9.4×10^{-5}, experimental (25° C)	4.5×10^{-17}, experimental (25° C)	1.1×10^{-4}, experimental (25° C)	6.3×10^{-6}, experimental (25° C)
Henry's Law Constant, atm-m^3/mole	2.1×10^{-2} experimental (25° C)	4.3×10^{-17}, experimental (25° C)	2.2, EPI estimated (25° C)	$8.0 \times 10^{-6,}$ EPI estimated (25° C)
Log Kow	7.7, experimental	6.0, experimental (25° C)	9.7, estimated(25° C)	7.45 , experimental
K_{oc}	15,000	247	3.9×10^5	62,000
Hydrolysis Photolysis	Based-catalyzed hydrolysis, half-life: 1 year; 10 years at pH7 Stable to photolysis	EPI can not estimate hydrolysis kinetics for this compound. Stable to direct photolysis in water	Based-catalyzed hydrolysis, half-life: ~ 10 months year; 9 years at pH7 Stable to direct photolysis in water	Based-catalyzed hydrolysis, half-life: 266 days; 7 years at pH7 No information on photolytic stability
Biodegradation (Expert Survey)	Ultimate (weeks) 3.0 Primary (days) 3.9	Ultimate (weeks) 3.3 Primary (days) 4.3	Ultimate (weeks) 3.1 Primary (days) 4.1	Ultimate (weeks) 2.98 Primary (days) 3.9
Fish Acute Toxicity, 96h-LC_{50}, ppm	$(0.07)^x$	acrylates $(1.2)^x$, esters $(0.45)^x$, vinyl/allyl alcohols $(1.18)^x$	0.004*	$(0.03)^x$
Fish Chronic, ppm	$(8.2 \times 10^{-4)})$	acrylates (0.003), esters	8.5×10^{-6}	(1.8×10^{-4})

Physical and Chemical Property	Isopropyl Miristate (C14) Tetradecanoic Acid, 1-methylethyl ester 110-27-0	Ascorbyl Palmitate (C16) L-Ascorbic acid, 6-hexadecanoate 137-66-6	Butyl Stearate (C18) Octadecanoic Acid, butyl ester 123-95-5	Methyl Oleate (C18) 9-Octadecenoic Acid (*Z*)-, methyl ester 112-62-9
Daphnia Acute Toxicity ,48-h-EC_{50}, ppm	(0.004)	acrylates $(0.36)^x$, esters $(0.07)^x$,	2.6×10^{-5}	(7.8×10^{-4})
Algae Toxicity, 96h-EC_{50}	(0.007)	acrylates (0.04), esters (0.04)	0.0004*	(0.003)
Mammal acute oral LD_{50} mg/kg			>32,000	
*Note chemical may not be soluble enough to result in the predicted effect				

Table 3- Continued **Fatty Acid Esters (C14- C18 fattyacids ; Saturated) and C-18 fatty acid, Unsaturated**

Physical and Chemical Property	Glyceryl Monostearate (C18) Octadecanoic acid, monoester with 1,2,3-propanetriol 31566-31-1
Number of carbon double bonds	One Can exist as *cis*- and *trans*-isomers
Water Solubility, mg/L	0.0123
Vapor Pressure, mmHg	1.27×10^{-9} estimated at 25° C
Henry's Law Constant, atm-m^3/mole	4.9×10^{-8} estimated at 25° C
Log Kow	6.62
K_{oc}	580
Hydrolysis Photolysis	Hydrolysis Based-catalyzed, 281.1 Neutral, 7.7 years Stable to direct photolysis

Physical and Chemical Property	**Glyceryl Monostearate (C18)** **Octadecanoic acid, monoester with 1,2,3-propanetriol** **31566-31-1**
Biodegradation (Expert Survey)	Ultimate (weeks), 3.1 Primary (days), 4.8
Fish Acute Toxicity, 96h-LC_{50}, ppm	0.18*
Fish Chronic Toxicity, ppm	0.003
Daphnia Acute Toxicity, 48h-EC_{50}	0.02*
Algae Toxicity, 96h-EC_{50}	0.02*
*Note chemical may not be soluble enough to result in the predicted effect	

Table 4- Derivatives of Fatty Acids (Not Esters), C16-C18 (Saturated) and C18 (Unsaturated)

Physical and Chemical Property	Sodium Oleyl Sulfate 9-Octadecen-1-ol, hydrogen sulfate, sodium salt 1847-55-8 C18	"Sulfonated Oleic Acid" C18 68443-05-0 Not in EPI or ECOSAR
Number of carbon double bonds	One Can exist as *cis*- and *trans*- isomers	
Water Solubility, mg/L	0.77, experimental (25° C)	
Vapor Pressure, mmHg	2.11×10^{-15}, experimental (25° C)	
Henry's Law Constant, atm-m^3/mole	1.32×10^{-15}, EPI estimated (25° C)	
Log Kow	4.42, experimental (25° C)	
K_{oc}	4.02×10^5	
Hydrolysis Photolysis	EPI can not estimate hydrolysis kinetics for this compound. Stable to direct photolysis in water	
Biodegradation (Expert Survey)	Ultimate (weeks) 2.7 Primary (days) 3.6	
Fish Acute Toxicity, 14 day LC_{50}, ppm	neutral organic (3.88)*	
*Note chemical may not be soluble enough to result in the predicted effect		

Table 5- **Alkali Metals, Alkali Earth Metals, and Ammonium Salts of Fatty Acids**

Physical and Chemical Property	Lauric Acid, Potassium Salt (12) 10124-65-9	Magnesium Stearate (C18)* Octadecanoic Acid, Magnesium Salt 557-04-0	Calcium Stearate* (C18) 1592-23-0	Ammonium Stearate (C18) Octadecanoic Acid, Ammonium Salt 1002-89-7
Number of carbon double bonds	None	None	None	None
Water Solubility, mg/L	1.19	1.0×10^{-10} at 25° C**	8.2×10^{-11} at 25° C**	0.56
Vapor Pressure, mmHg	1.5×10^{-10}, estimated (25° C)	$6.5 \times 10^{-15,}$ estimated at 25° C	$4.5 \times 10^{-14,}$ estimated at 25° C	2.5×10^{-8} estimated at 25° C
Henry's Law Constant, atm-m^3/mole	1.8×10^{-18}, estimated (25° C)	$4.8 \times 10^{-5,}$ estimated at 25° C	$4.3 \times 10^{-4,}$ estimated at 25° C	$1.8 \times 10^{-8,}$ estimated at 25° C
Log Kow	1.19	14.4	14.3	5.1
K_{oc}	296	9.2×10^8	9.2×10^8	8.0×1^4
Hydrolysis Photolysis	No data available	Stable to hydrolysis and direct photolysis	Stable to hydrolysis and direct photolysis	Base-catalyzed hydrolysis half-life, 6.9 days; 69 days at neutral pH Stable to direct photolysis
Biodegradation (Expert Survey)	Ultimate (weeks), 2.9 Primary (days), 387	Ultimate (weeks), 2.5 Primary (days), 3.5	Ultimate (weeks), 2.5 Primary (days), 3.5	Ultimate (weeks), 2.8 Primary (days), 3.7
Fish Acute Toxicity, 96h-LC_{50}, ppm	neutral organic (1625)* (14 day)	neutral organic (1.1×10^{-9})*	neutral organic (1.13×10^{-9})*	neutral organic (0.86)* (14 day)
Fish Chronic Toxicity, 30 day, ppm		neutral organic (1.04×10^{-9})*	neutral organic (1.04×10^{-9})*	
Daphnia Acute Toxicity, 48h-EC_{50}, ppm		neutral organic (2.77×10^{-9})*	neutral organic (2.84×10^{-9})*	
Mysid Shrimp Toxicity, 96h-LC_{50}, ppm		neutral organic (4.75×10^{-14})	neutral organic (4.88×10^{-14})	
Algae Toxicity, 96h-EC_{50},		neutral organic (3.52×10^{-9})*	neutral organic (3.62×10^{-9})*	

Physical and Chemical Property	Lauric Acid, Potassium Salt (12) 10124-65-9	Magnesium Stearate (C18)* Octadecanoic Acid, Magnessium Salt 557-04-0	Calcium Stearate* (C18) 1592-23-0	Ammonium Stearate (C18) Octadecanoic Acid, Ammonium Salt 1002-89-7
Bobwhite quail acute oral LD_{50}, mg\kg				2150 (14.65% test material)
Note* chemical may not be soluble enough to result in the predicted effect				

Table 6. Aluminum and Zinc Stearates

Physical and Chemical Property	Aluminum Stearate* Aluminum Tristearate 637-12-7	Zinc Stearate** 557-05-1
Number of carbon double bonds	None	None
Water Solubility, mg/L	9.4×10^{-20}, at 25° C	4.6×10^{-11}, at 25° C
Vapor Pressure, mmHg	1.0×10^{-18}, estimated at 25° C	2.7×10^{-15}, estimated at 25° C
Henry's Law Constant, atm-m^3/mole	1.2×10^{-4}, estimated at 25° C	4.9×10^{-5}, estimated at 25° C
Log Kow	22.7	14.4
K_{oc}	1×10^{10}	9.2×10^{8}
Hydrolysis Photolysis	Stable to hydrolysis and direct photolysis	Stable to hydrolysis and direct photolysis
Biodegradation (Expert Survey)	Ultimate (weeks), 2.2 Primary (days), 3.4	Ultimate (weeks), 2.4 Primary (days), 3.5
Fish Acute Toxicity, 96h-LC_{50} ppm	neutral organic (2.32×10^{-17})*	neutral organic (9.49×10^{-10})*
Fish Chronic Toxicity, 30 day, ppm	neutral organic (8.37×10^{-17})*	neutral organic (9.08×10^{-10})*
Daphnia Acute Toxicity, 48h- EC50, ppm	neutral organic (1.04×10^{-16})*	neutral organic (2.4×10^{-9})*
Mysid Shrimp Toxicity, 96h-LC_{50}, ppm	neutral organic (2.57×10^{-24})	neutral organic (4.75×10^{-14})
Algae Toxicity, 96h-EC_{50}, ppm	neutral organic (2.13×10^{-16})*	neutral organic (3.52×10^{-9})*
Mammal acute oral LD_{50}, mg/kg		>10,000
Note* chemical may not be soluble enough to result in the predicted effect		

* Also included under "Salts of fatty acids, conforming to 21 CFR 172.863"

** Zinc stearate prepared from stearic acid free chick-edema factor (Zinc stearate, conforming to 21 CFR 182.5994 and 582.5994)